

=> d his ful

(FILE 'HOME' ENTERED AT 20:40:36 ON 20 MAR 2010)

INDEX 'ABI-INFORM, ADISCTI, ADISINSIGHT, ADISNEWS, AQUALINE, AQUASCI, BIOENG, BIOSIS, BIOTECHNO, CAPLUS, CBNB, CHEMLIST, CIN, CONFSCI, CSNB, DISSABS, EMBAL, EMBASE, ENERGY, ENVIROENG, ESBIODEBASE, FOMAD, FROSTI, HEALSAFE, HSDB, IFIPAT, INIS, IPA, KOSMET, ...' ENTERED AT 20:41:29 ON 20 MAR 2010

FILE 'REGISTRY' ENTERED AT 20:41:56 ON 20 MAR 2010

L1 0 SEA PLU=ON FLURO AND DIMETHYL AND TRIMETHYLBUTYL AND PHENYL AND PYRAOZLE AND CARBOXAMIDE
L2 0 SEA PLU=ON FLURO AND DIMETHYL AND TRIMETHYLBUTYL AND PHENYL AND PYRAZOLE AND CARBOXAMIDE
L3 0 SEA PLU=ON FLURO AND DIMETHYL AND TRIMETHYLBUTYL AND PHENYL AND CARBOXAMIDE
L4 0 SEA PLU=ON FLURO AND DIMETHYL AND METHYL AND BUTYL AND PHENYL AND CARBOXAMIDE
L5 0 SEA PLU=ON FLURO AND DIMETHYL AND METHYL AND BUTYL AND PHENYL AND CARBOX AND AMIDE
L6 4914 SEA PLU=ON FLUORO AND DIMETHYL AND METHYL AND BUTYL AND PHENYL AND CARBOX AND AMIDE
L7 13 SEA PLU=ON FLUORO AND DIMETHYL AND TRIMETHYLBUTYL AND PHENYL AND PYRAZOLE AND CARBOXAMIDE
D 1-
L8 1 SEA PLU=ON 494793-45-2
L9 6 SEA PLU=ON 494793-45-2 OR 494793-45-2/CRN
L10 0 SEA PLU=ON DIMETHYLBUTYL AND PHENYL AND FLUORO AND DIMETHYL AND PYRAZOLE AND CARBOXAMIDE
L11 554 SEA PLU=ON DIMETHYLBUTYL AND PHENYL AND FLUORO AND DIMETHYL AND PYRAZOLE AND CARBOXAMIDE
L12 0 SEA PLU=ON L1 AND 1H
L13 479 SEA PLU=ON L11 AND 1H
L14 472 SEA PLU=ON L13 AND PYRAZOLE-4-CARBOXAMIDE
L15 438 SEA PLU=ON L14 AND 1,3-DIMETHYLBUTYL
L16 438 SEA PLU=ON L14 AND "1,3-DIMETHYLBUTYL"
L17 104 SEA PLU=ON L14 AND "1,3-DIMETHYLBUTYL" (5A) 5-FLUORO
L18 104 SEA PLU=ON L14 AND "1,3-DIMETHYLBUTYL" (5A) 5-FLUORO (5A)
1,3-DIMETHYL
L19 104 SEA PLU=ON L14 AND "1,3-DIMETHYLBUTYL" (5A) 5-FLUORO (5A)
1,3-DIMETHYL (5A) 1H-PYRAZOLE-4-CARBOXAMIDE
L20 104 SEA PLU=ON L14 AND "2" (5A) "1,3-DIMETHYLBUTYL" (5A) 5-FLUORO (5A) 1,3-DIMETHYL (5A) 1H-PYRAZOLE-4-CARBOXAMIDE
L21 104 SEA PLU=ON L14 AND N (5A) "2" (5A) "1,3-DIMETHYLBUTYL" (5A)
5-FLUORO (5A) 1,3-DIMETHYL (5A) 1H-PYRAZOLE-4-CARBOXAMIDE
L22 34 SEA PLU=ON "N-[2-(1,3-DIMETHYLBUTYL)PHENYL]-5-FLUORO-1,3-DIMET
HYL-1H-PYRAZOLE-4-CARBOXAMIDE"
D 1-
L23 106 SEA PLU=ON 494793-67-8/CRN OR 494793-67-8
L24 0 SEA PLU=ON "N-[2-(1,3-DIMETHYLBUTYL)PHENYL]-2-TRIFLUORO)BENZAM
IDE"
L25 11 SEA PLU=ON "N-[2-(1,3-DIMETHYLBUTYL)PHENYL]-2-TRIFLUORO)" AND
BENZAMIDE
D 1-
L26 11 SEA PLU=ON 640290-16-0/CRN OR 640290-16-0
L27 3 SEA PLU=ON "N-[2-(1,3-DIMETHYLBUTYL)PHENYL]" AND 2-IODOBENZAM
IDE
D 1-
L28 9 SEA PLU=ON 640290-17-1 OR 640290-17-1/CRN

L29

132 SEA PLU=ON L9 OR L23 OR L26 OR L28

INDEX 'ABI-INFORM, ADISCTI, ADISINSIGHT, ADISNEWS, AQUALINE, AQUASCI, BIOENG, BIOSIS, BIOTECHNO, CAPLUS, CBNB, CHEMLIST, CIN, CONFSCI, CSNB, DISSABS, EMBAL, EMBASE, ENERGY, ENVIROENG, ESBIOWBASE, FOMAD, FROSTI, HEALSAFE, HSDB, IFIPAT, INIS, IPA, KOSMET, ...' ENTERED AT 20:56:55 ON 20 MAR 2010

SEA L29

0* FILE ABI-INFORM
0* FILE ADISCTI
0* FILE ADISINSIGHT
0* FILE ADISNEWS
0* FILE AQUALINE
0* FILE AQUASCI
0* FILE BIOENG
0* FILE BIOSIS
0* FILE BIOTECHNO
88* FILE CAPLUS
0* FILE CBNB
0* FILE CHEMLIST
0* FILE CIN
0* FILE CONFSCI
0* FILE CSNB
0* FILE DISSABS
0* FILE EMBAL
0* FILE EMBASE
0* FILE ENERGY
0* FILE ENVIROENG
0* FILE ESBIOWBASE
0* FILE FOMAD
0* FILE FROSTI
0* FILE HEALSAFE
0* FILE HSDB
0* FILE IFIPAT
0* FILE INIS
0* FILE IPA
0* FILE KOSMET
0* FILE LIFESCI
0* FILE MEDLINE
0* FILE MSDS-CCOHS
0* FILE MSDS-OHS
0* FILE NAPRALERT
0* FILE NLDB
0* FILE NTIS
0* FILE PASCAL
0* FILE POLLUAB
0* FILE PROMT
0* FILE RTECS
0* FILE SCISEARCH
19* FILE TOXCENTER
0* FILE USPATFULL
0* FILE USPAT2
0* FILE WATER
0* FILE DDFB
0* FILE DDFU
0* FILE DGENE
0* FILE DRUGB
0* FILE DRUGMONOG2
0* FILE DRUGU
0* FILE IMSDRUGNEWS

0* FILE IMSPRODUCT
0* FILE PCTGEN
0* FILE USGENE
0* FILE USPATOLD
0* FILE BABS
0* FILE EPFULL
0* FILE IMSPATENTS
0* FILE IMSRESEARCH
0* FILE PCTFULL
0* FILE PROUSDDR
0* FILE PS
0* FILE RDISCLOSURE
0* FILE SYNTHLINE
0* FILE USAN
0* FILE AGRICOLA
0* FILE ANTE
0* FILE CABA
0* FILE CROPB
0* FILE CROPU
0* FILE FSTA
0* FILE GENBANK
L30 QUE PLU=ON L29

FILE 'CAPLUS, TOXCENTER' ENTERED AT 20:57:28 ON 20 MAR 2010
L31 118 SEA PLU=ON L30
L32 99 DUP REM L31 (19 DUPLICATES REMOVED)
 D 1- BIB,AB,HITSTR

INDEX 'ABI-INFORM, ADISCTI, ADISINSIGHT, ADISNEWS, AQUALINE, AQUASCI,
BIOENG, BIOSIS, BIOTECHNO, CAPLUS, CBNB, CHEMLIST, CIN, CONFSCI, CSNB,
DISSABS, EMBAL, EMBASE, ENERGY, ENVIROENG, ESBIOBASE, FOMAD, FROSTI,
HEALSAFE, HSDB, IFIPAT, INIS, IPA, KOSMET, ...' ENTERED AT 21:00:15 ON 20
MAR 2010

FILE 'REGISTRY' ENTERED AT 21:34:30 ON 20 MAR 2010
L33 STRUCTURE uploaded
L34 26 SEA SSS SAM L33
 D 1-
L35 426 SEA SSS FUL L33

INDEX 'ABI-INFORM, ADISCTI, ADISINSIGHT, ADISNEWS, AQUALINE, AQUASCI,
BIOENG, BIOSIS, BIOTECHNO, CAPLUS, CBNB, CHEMLIST, CIN, CONFSCI, CSNB,
DISSABS, EMBAL, EMBASE, ENERGY, ENVIROENG, ESBIOBASE, FOMAD, FROSTI,
HEALSAFE, HSDB, IFIPAT, INIS, IPA, KOSMET, ...' ENTERED AT 21:42:52 ON 20
MAR 2010

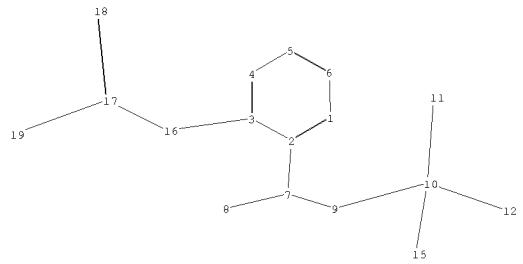
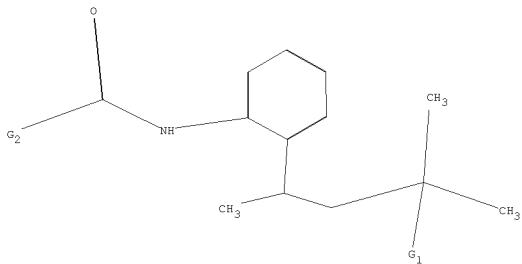
SEA L35

0* FILE ABI-INFORM
0* FILE ADISCTI
0* FILE ADISINSIGHT
0* FILE ADISNEWS
0* FILE AQUALINE
0* FILE AQUASCI
0* FILE BIOENG
0* FILE BIOSIS
0* FILE BIOTECHNO
0* FILE CAPLUS
0* FILE CBNB
0* FILE CHEMLIST
0* FILE CIN

0* FILE CONFSCI
0* FILE CSNB
0* FILE DISSABS
0* FILE EMBAL
0* FILE EMBASE
0* FILE ENERGY
0* FILE ENVIROENG
0* FILE ESBIOBASE
0* FILE FOMAD
0* FILE FROSTI
0* FILE HEALSAFE
0* FILE HSDB
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0* FILE KOSMET
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0* FILE MSDS-OHS
0* FILE NAPRALERT
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0* FILE SCISEARCH
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0* FILE DDFB
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0* FILE DGENE
0* FILE DRUGB
0* FILE DRUGMONOG2
0* FILE DRUGU
0* FILE IMSDRUGNEWS
0* FILE IMSPRODUCT
0* FILE PCTGEN
0* FILE USGENE
0* FILE USPATOLD
0* FILE BABS
0* FILE EPFULL
0* FILE IMSPATENTS
0* FILE IMSRESEARCH
0* FILE PCTFULL
0* FILE PROUSDDR
0* FILE PS
0* FILE RDISCLOSURE
0* FILE SYNTHLINE
0* FILE USAN

L36 QUE PLU=ON L35

FILE 'CAPLUS' ENTERED AT 21:43:13 ON 20 MAR 2010
L37 131 SEA PLU=ON L35
L38 131 DUP REM L37 (0 DUPLICATES REMOVED)
 D 1- BIB,AB,HITSTR



chain nodes :
 7 8 9 10 11 12 15 16 17 18 19

ring nodes :

1 2 3 4 5 6

chain bonds :

2-7 3-16 7-8 7-9 9-10 10-11 10-12 10-15 16-17 17-18 17-19

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

3-16 10-15 16-17 17-18 17-19

exact bonds :

2-7 7-8 7-9 9-10 10-11 10-12

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

G1:H,CH3,CH2,CH,Et,n-Pr,i-Pr,CF2,CF3,CCl2,CCl3,CBr2,CBr3,X,Ak

G2:Cb,Hy

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS
 12:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS